Project: ace175

2022 DOE Vehicle Technologies Office Annual Merit Review

Co-optimization of fuel physical/chemical properties and combustion system for mixing controlled compression ignition (MCCI) in a medium-duty engine

Flavio Chuahy (PI)

Corey Trobaugh (Cummins Co-PI)

Oak Ridge National Laboratory

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This presentation does not contain any proprietary, confidential, or otherwise restricted information

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Overview

Timeline

- **Program awarded in May 2021**
- **Program approved March 29th, 2022**
- **Program duration of 18 months**
- **Program is 5% complete to date**

Budget

Total Project Funding $312,500

Task	Budget
ORNL	$250K
Cummins (in-kind)	$62.5K

Barriers

21st Century Truck Roadmap

- **Drive efficiency towards 60% for MD** & HD powertrains
- Internal Combustion Engine Powertrain: Reduction of combustion heat losses + Combustion system improvements.
- Co-optimization of the fuel with engine combustion categories.

Co-Optimization of Fuels and Engines

- **Better fuels. Better Engines. Sooner**

Partners

- **Formal partners**
  - Cummins (CRADA Partner)
- **Informal partners**
  - Lawrence Berkeley National Laboratory

Relevance

Overall Co-Optima Goal — **Better fuels, better vehicles, faster**

The objective of this project is to co-optimize fuel properties and engine/fuel-system geometry to demonstrate the potential changes to fuel formulations and combustion system architectures that may improve CO_2, engine efficiency and other pollutant emissions.

Taking advantage of the central fuel hypothesis — **Equivalent fuel properties will result in equivalent performance**

- **Physical properties will be optimized in tandem with injector geometry, injection strategy and piston bowl geometry for two relevant fuel chemistries, conventional 45 cetane diesel fuel and hydrotreated vegetable oil (HVO)**

- Increased HVO utilization in this sector improves energy security through energy diversification and available known national resources

- **Reduced GHG emissions through fuel properties and efficiency improvements**

Fully coupled fuel and engine co-optimization in a medium-duty engine platform using advanced optimization algorithms.

Milestones for FY22/23

Milestone	Due Date	Status
Define fuel property, fuel system and piston geometry ranges	6/30/2022 (3 months)	**Completed**
Couple and test black box advanced optimizer with CAESES and CONVERGE CFD engine model	9/31/2022 (6 months)	On-Track
Develop fuel surrogate for Hydrotreated Vegetable Oil fuel (HVO)	12/31/2022 (9 months)	On-Track
Deliver results of optimization for 45 cetane conventional diesel fuel	3/30/2023 (12 months)	On-Track
Deliver results of optimization for HVO fuel	9/30/2023 (18 months)	On-track

Any proposed future work is subject to change based on funding levels.

Optimization includes combustion system geometry (piston and injector), fuel physical properties and injection strategy

- Objective Function: Engine indicated efficiency

- Constraints
  - NOx emissions
  - CO emissions
  - HC emissions
  - PAH emissions as a surrogate for soot
  - Mechanical constraints

- A large number of variables are included in the optimization:

Fuel Physical Properties	Fuel System Design	Bowl Geometry	Injection Strategy	Fuel Chemical Composition
Liquid density	Spray angle	Fully parametrized bowl design → Compression ratio	Injection Pressure	High aromatic diesel (Conventional diesel)
Liquid viscosity	Nozzle protrusion		Injection Timings (three injections)	Low aromatic diesel, highly paraffinic fuel (HVO)
Heat of vaporization	Nozzle diameter		Injection Durations	
Surface tension				

- Cummins to set appropriate limits to each variable
- Engine operating condition will be chosen based on representative operating point from a MD duty cycle.

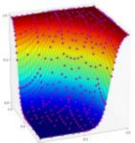
Integrated optimization approach using state-of-the-art algorithms and software

Two fuel chemistries

Diesel

HVO

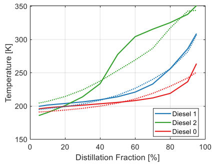
Black Box Global Optimization



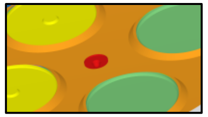
Machine Learning (ML) assisted optimization

Creation of CFD Cases

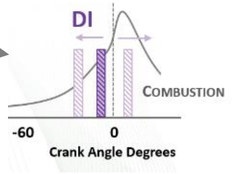
Fuel Physical Properties



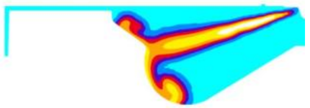
Injector Geometry



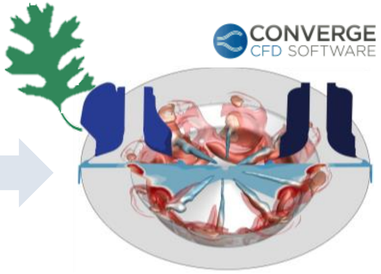
Injection Strategy



Bowl Geometry



Combustion CFD

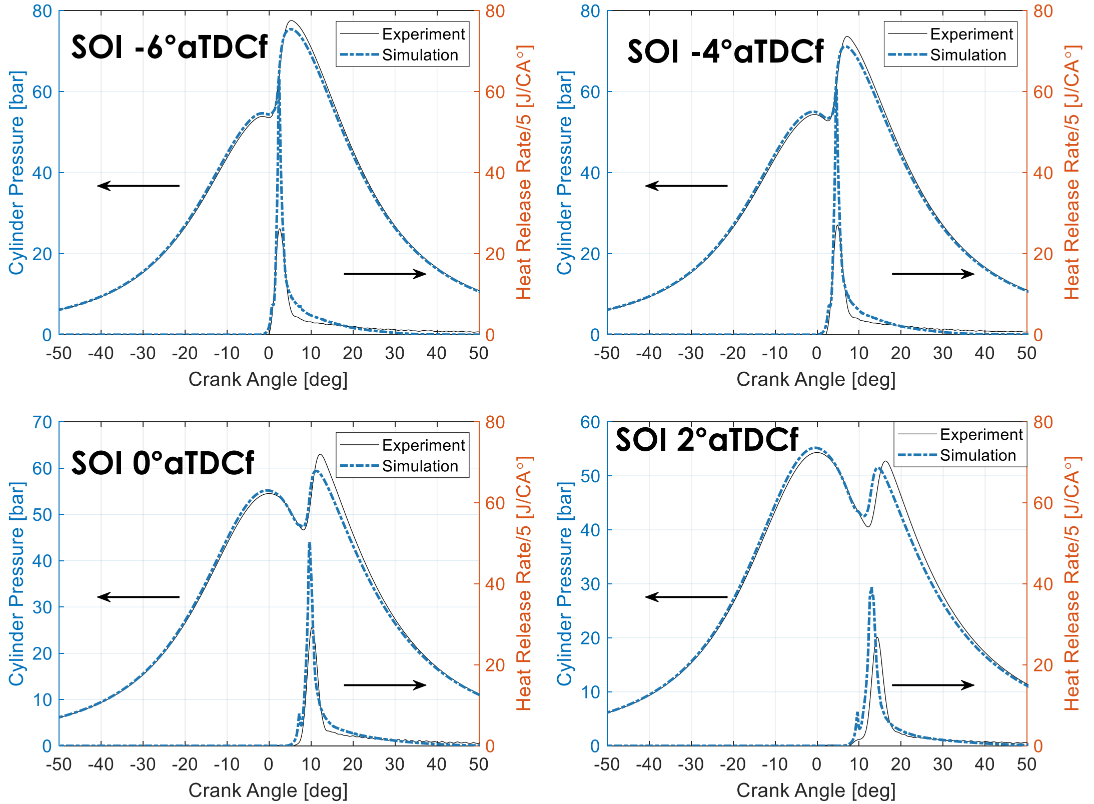


Model Training and New Search

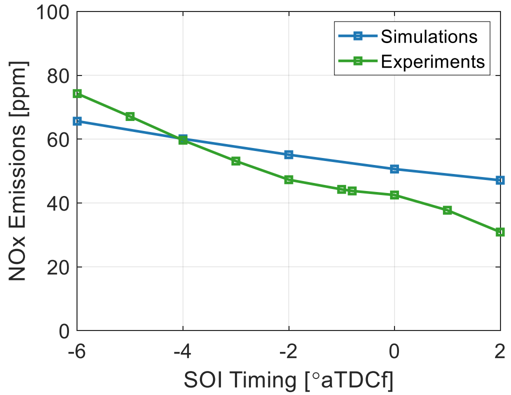
CAESES Post Processing:
- Emissions index calculations
- Efficiency calculations
- Constraints (Peak cylinder pressure, etc.)

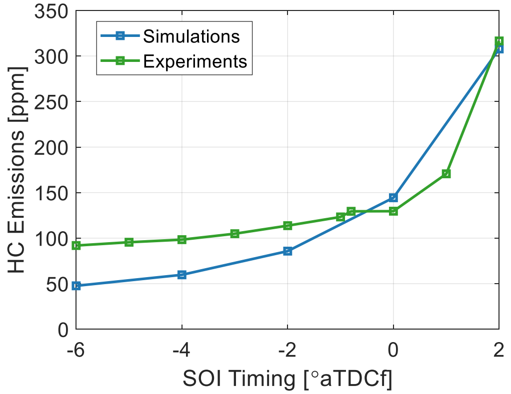
Standing on the shoulders of Co-Optima core program work. Engine model developed and validated.

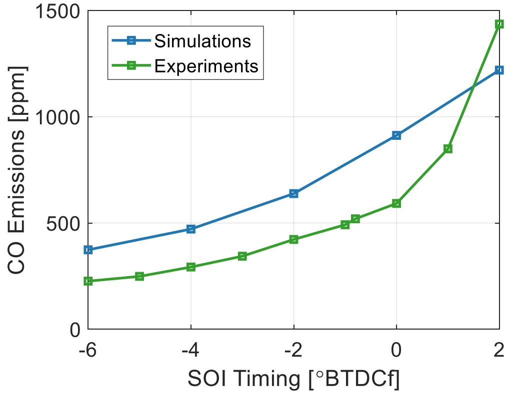
- Model validated @ 3.8 bar IMEPg condition across a start of injection (SOI) sweep using **Diesel #1**.
- Heat release rate is well captured for all SOI conditions without independent tuning of cases.
- NOx, CO and unburned HC emission trends and magnitude are well captured by the model.
- Mechanism includes PAH, Thermal NOx and Prompt NOx
- PAH formation will be used as surrogate for soot formation → Not currently coupled with soot model.



	Cummins ISB
Bore (mm)	107
Stroke (mm)	124
Connecting rod (mm)	192
Compression ratio(-)	20
Displacement per cylinder (l)	1.16







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Collaboration and Coordination with Other Institutions

- This program is a collaborative project between Cummins and ORNL. Program will leverage on-road and off-road experience from Cummins as part of their own research activities. This combines industry experience and world-class DOE computing expertise to assess the potential for substantial efficiency gains in compression ignition engines relevant to medium duty through co-optimization of fuel properties and engine geometry.

- The work plan for this program was developed following roadmaps for 21st Century Truck partnership and Co-optima core goals.

- Leveraging stakeholder feedback from AEC MOU member companies (15 members)

- Individual collaborations for this project:
  - **Cummins** – CRADA Partner: Provide guidance on design parameters and experience.
  - **Lawrence Berkeley National Laboratory** – Informal Collaborator: Will provide access to advanced black-box optimization algorithms.

Any proposed future work is subject to change based on funding levels.

Proposed Future Research

FY22

I. **Cummins to define optimization Parameter Ranges:**
   I. Decision on bowl shape parametrization and range
   II. Decision on ranges for fuel physical properties
   III. Decision on ranges for injector geometrical features
   IV. Decision on ranges for injection strategies including 3 injections.
II. **Integrate Advanced Optimizer with CAESES and ORNL cluster**
   I. Integrate and test the functionality of the automated optimization process.
III. **Optimization of CFD run time**

FY23

I. **Develop fuel surrogate for HVO fuel:**
   I. Develop surrogate for high paraffinic fuel and review with Cummins
II. **Conduct optimization for conventional 45 cetane number diesel fuel**
   I. Assessment of capabilities of chosen optimization approach
   II. Study of parametric effects and sensitivity to design parameters
   III. Analysis of Pareto frontier of possible piston, fuel and injector designs.
III. **Conduct optimization for HVO fuel**
   I. Comparison to conventional diesel results.
   II. Contrast fuel property effects between the different chemistries.
IV. **Cummins to assess feasibility of piston designs and proposed fuel compositions**

Summary

Relevance

- Program is in line with 21st Century Truck partnership research roadmap of increasing medium duty diesel combustion efficiency. Focusing on co-optimization of combustion system architecture and fuel properties.
- Program is in line with core Co-Optimization of Fuels and Engines goal of achieving better fuels and better engines, faster.

Approach

- Optimization of engine efficiency under emissions constraints.
- Combination of an advanced black-box global optimizer with detailed combustion CFD to co-optimize fuel properties and combustion system architecture simultaneously.

Collaborations

- Collaboration with Cummins (CRADA partner) and Lawrence Berkeley National Laboratory (informal)

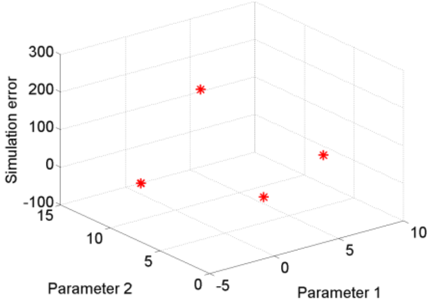
Future Work

- Cummins to set limits for optimization parameters and determine operating condition of interest based on MD duty cycle.
- Conduct optimization for conventional 45 cetane number diesel fuel
- Conduct optimization for HVO fuel
- Contrast effects of physical properties on both fuels, and its impact on chosen geometry design.
- Cummins to analyze feasibility of proposed designs and fuel compositions.

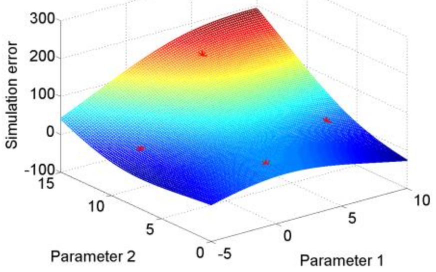
Technical Back-Up Slides

Optimizer uses a surrogate model to search for new promising data points

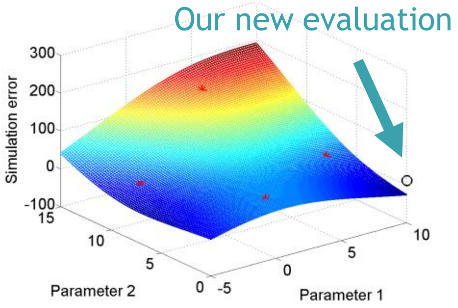
Initial experimental design

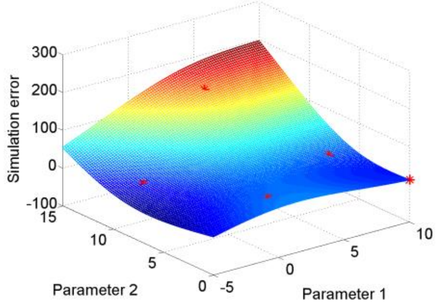


Create surrogate model

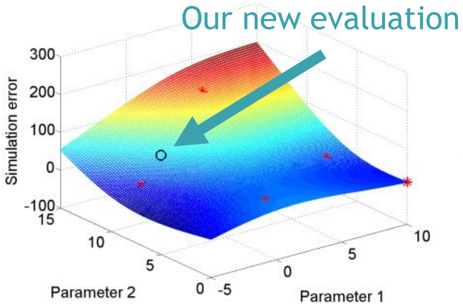


Select new evaluation point and evaluate the functions





Update the surrogate model with the new data point



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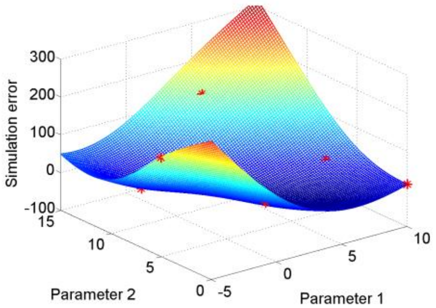

Update the surrogate model with the new data point

Radial Basis Functions for surrogate:

- Interpolating, only needs input-output data pairs
- Fast to build (solve linear system) and evaluate (matrix*vector)
- Work great for 20+ dimensions
- Work great for mixed-integer parameters (some continuous, some integers)
- Great flexibility for developing new sampling methods (e.g., constrained problems)

Previous Co-optima work is basis for new work with Cummins

- **Prior work developed the base model for this program**
- Detailed chemical mechanism developed by LLNL to be used with 319 species and 1797 reactions → Includes NOx (thermal and prompt) and PAH chemistry
- Model was validated for diesel #1 against single-cylinder experiments. Good agreement in heat release rate and emissions.

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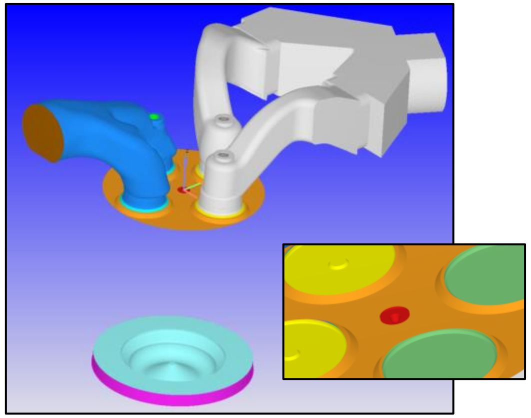
CONVERGE CFD Model



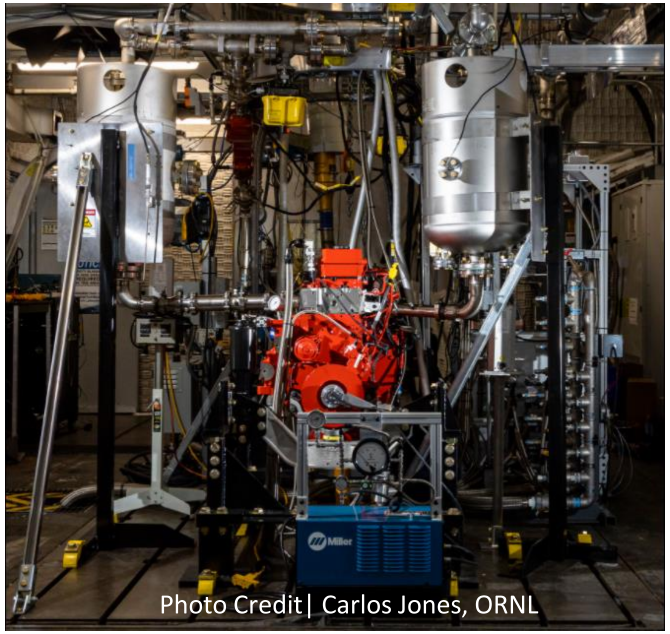


Photo Credit| Carlos Jones, ORNL

Computational Setup using CONVERGE 3.0

- Model created from laser scanned cylinder head, pistons and valves.
- Injector tip X-ray CT scanned for nozzle size and orientation validation as well as geometry. (nominal 141um 145° included angle)
- Injection rate shapes sourced from Bosch bench injection rate data
- Step lipped bowl with 20:1 compression ratio.
- Resulting mechanism 319 species 1797 reactions → Including PAH and NOx chemistry

CFD Software	Converge 3.0.18
Fuel Injection	Blob
Droplet Break-up	KH-RT
Droplet Collision	NTC
Droplet Drag	Dynamic
Droplet Evaporation	Frossling Correlation
Combustion	SAGE w/ adaptive zoning
Turbulence	RNG k-epsilon
Base mesh size in cylinder	1 mm
Adaptive mesh refinement (AMR) cell size based on temperature and velocity	0.25 mm
Peak Cell Count	~2M Cells

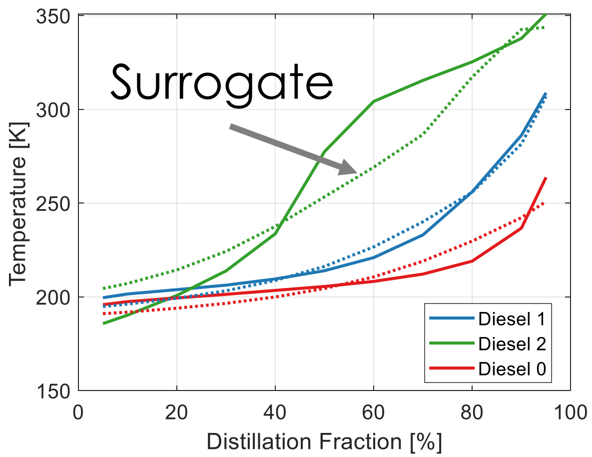
OEMs can have access to the mechanism by contacting kukkadapu1@llnl.gov or pitz1@llnl.gov

Surrogates Developed for Each Diesel Fuel

- 5 component surrogate fuels developed for each diesel fuel.
- H/C ratio, density, DCN and distillation curve targeted in optimization

	Diesel #2	Diesel #1	Diesel #0
Density [kg/m3]	844.4	827.0	816.2
H/C Ratio [-]	1.864	1.855	1.892
Cetane Number [-]	45.3	45.3	45.4
Aromatic Content [%vol]	15.1	15.6	14.4
Olefin Content [%vol]	1.0	0.6	0.6
Saturate Content [%vol]	83.8	83.8	85
Kinetic Viscosity [cst]	2.88	1.74	1.44

- Co-Optima work on diesel surrogates will be leveraged as a starting point for conventional 45 cetane number diesel fuel.



* Surrogates designed at LLNL using tool developed by Russell Whitesides.